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UNIVERSITY of PENNSYLVANIA

School of Engineering and Applied Science
Department of Materials Science and Engineering
Philadelphia, PA 19104-6272
Takeshi Egami
Professor

July 28, 1992

Grant Administration
Office of Naval Research
Arlington, VA 22217

RE: FY 90 Report

Dear Sir:

Enclosed please find copies of the FY90 end of the year report which was filed but apparently was not distributed properly. Thank you for your attention.

Sincerely yours,

T. Egami

FY91 End of Fiscal Year Letter
(01 Oct 1990 - 30 Sep 1991)

ONR CONTRACT INFORMATION

Contract Title: Atomic Structure of Mixed Ferroelectrics

Performing Organization: University of Pennsylvania

Principal Investigator: Dr. Takeshi Egami

Contract Number: N00014-91-J-1036

R & T Project Number:

ONR Scientific Officer: Dr. Wallace A. Smith

Enclosure (1)

Statement A per telecon Wallace Smith
ONR/Code 1131
Arlington, VA 22217-5000

NWW 8/19/92

A. Research Goals.

The purpose of this project is to determine the local atomic structure of mixed ferroelectric solids such as $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN) by diffraction experiments, in order to obtain better understanding of the basis for their relaxor ferroelectric behavior. In particular we use pulsed neutron and synchrotron x-ray scattering measurements, and analyze the results in terms of the atomic pair distribution function.

B. Significant results.

1. Anomalous scattering study

Anomalous x-ray scattering measurements were carried out for PMN at the Nb K-edge. The x-ray scattering intensity of an element depends strongly upon energy near the absorption edge, due to the anomalous dispersion effect. By making use of this phenomenon it is possible to differentiate contributions from different elements to the total scattering intensity. This technique is called the x-ray anomalous scattering study. The experiment was carried out at X-7A beamline of the National Synchrotron Light Source (NSLS) of Brookhaven National Laboratory. The result indicates that the Nb atoms are located in the b.c.c. positions, which include both A and B sites. This result has profound implications, overturning the conventional wisdom that Nb occupies only the A site. The data are being further analyzed with utmost care.

1. Temperature dependence of pair distribution function

In another set of experiments at the NSLS, the x-ray scattering from a powder sample of PMN was measured as a function of temperature around the ferroelectric freezing temperature. The data were corrected for absorption and other effects, and were Fourier-transformed to obtain the atomic pair distribution function (PDF) which describes the distribution of the interatomic distances. The results show significant changes in the atomic short range order even above the freezing temperature.

C. Plans for the Next Year's Research

The results obtained for PMN last year as described above are quite significant and underscore our belief on the importance of studying the atomic short range order in understanding this material. However, the results are somewhat preliminary, and the subject needs to be more thoroughly studied. The goal of this year's research is to expand on the results we obtained, namely to carry out much more of the same type of experiments, and build a better structural model of PMN. More specifically;

1. We will carry out the anomalous x-ray scattering experiment of PMN also at the Pb edge, in addition to the Nb edge as we already did. This will be a crucial test whether Pb atoms are both on the A and B sites, as the Nb edge results suggested.

2. The PDF of PMN will be determined over a wider temperature range, down to 10 K, and up to 600 K.

3. The atomic structure of PMN will be modelled by the Monte-Carlo refinement procedure using both the x-ray and neutron PDF's.

This will involve at least three trips to the NSLS to carry out synchrotron x-ray scattering measurements.

D. List of Publications/Reports/Presentations

1. Papers Published in Refereed Journals

"Diffraction Studies of Local Atomic Structure in Ferroelectric and Superconducting Oxides", T. Egami, H. D. Rosenfeld, B. H. Toby and A. Bhalla, Ferroelectrics, 120, 11 (1991).

2. Non-Refereed Publications and Published Technical Reports

None

3. Presentations

a. Invited

"Diffraction Studies of Local Atomic Structure in Ferroelectric and Superconducting Oxides", in ONR workshop at Williamsburg, Feb., 1991.

b. Contributed

None

4. Books (and sections thereof)

None

Enclosure (2)

E. LIST OF HONORS/AWARDS

Name of Person Receiving Award	Recipient's Institution	Name, Sponsor and Purpose of Award
None		

F. Participants

Principal Investigator: Dr. T. Egami

Postdoctoral Fellow : Dr. B. H. Toby, now at Air-Products Inc.

G. Other Grants

1. Title : Local Atomic Structure of Non-Crystalline Solids
   Sponsor : National Science Foundation
   Amount : $ 122,600 per annum
   Effort : 1 month of P.I.'s time
   Duration : May 15, 1990 - May 14, 1993

2. Title : Non-Periodic Structure of Matter
   Sponsor : National Science Foundation, Matrials Research Laboratory
   Amount : $ 64,924 per annum
   Effort : 0.5 mo. P.I.
   Duration : March 1, 1991 - Feb. 28, 1992

3. Title : Atomistic Study of Magneto-Optical Thin Films
   Sponsor : IBM, Shared University Research Program
   Amount : $ 84,300
   Effort : 1 mo. P.I.
   Duration : Jan.1, 1991 - Dec. 31, 1991

H. SUMMARY OF FY91
PUBLICATIONS/PATENTS/PRESENTATIONS/HONORS/PARTICIPANTS
(Number Only)

		ONR	non ONR
a.	Number of Papers Submitted to Referred Journal but not yet published:	0	8
b.	Number of Papers Published in Refereed Journals:	1	10
c.	Number of Books or Chapters Submitted but not yet Published:	0	0
d.	Number of Books or Chapters Published:	0	0
e.	Number of Printed Technical Reports & Non-Referred Papers:	0	0
f.	Number of Patents Filed:	0	0
g.	Number of Patents Granted:	0	0
h.	Number of Invited Presentations at Workshops or Prof. Society Meetings:	1	5
i.	Number of Contributed Presentations at Workshops or Prof. Society Meetings:	0	7
j.	Honors/Awards/Prizes for Contract/Grant Employees: (selected list attached)	0	0
k.	Number of Graduate Students and Post-Docs Supported at least 25% this year on contract grant:	1	7
	Grad Students: TOTAL	0	5
	Female	0	0
	Minority	0	0
	Post Doc: TOTAL	1	2
	Female	0	0
	Minority	0	0
l.	Number of Female or Minority PIs or CO-PIs		
	New Female	0	0
	Continuing Female	0	0
	New Minority	0	0
	Continuing Minority	1	1